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NEWS

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NEWS

This column regularly reports significant developments in the program of the National Standard Reference Data System, which was established to make critically evaluated data in the physical sciences available to science and technology on a national basis. The System is administered and coordinated by the NBS Office of Standard Reference Data.

Data Activities in West Germany

For many years the evaluation and compilation of data on the properties of substances have been a cooperative activity among the world's scientists. Two well known international compilations are the International Critical Tables and the Landolt-Börnstein Tables. While the former was an international undertaking from the beginning, the latter began as an entirely German effort.

To acquaint readers with some of these international efforts, *NSRDS News* has described such programs. The following description of data activities in West Germany was provided by Herbert Stussig, Vice Chairman, Federal Republic of Germany National Committee for CODATA.

Germany, with a long tradition in compiling and critically evaluating data, has produced four well known handbooks: Landolt-Börnstein's *Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik* (Numerical Data and Functional Relationships in Physics, Chemistry, Astronomy, Geophysics and Technology); Gmelin's *Handbuch der Anorganischen Chemie* (Handbook of Inorganic Chemistry); Beilstein's *Handbuch der Organischen Chemie* (Handbook of Organic Chemistry); and Ullman's *Encyklopädie der Technischen Chemie* (Encyclopedia of Technical Chemistry).

There are fundamental differences in the organization of the four handbooks. The Landolt-Börnstein tables are arranged according to the physical properties of the different materials and substances, whereas the Gmelin and the Beilstein handbooks are organized according to chemical substances. The Ullman encyclopedia essentially covers both aspects, but emphasizes technological application.

The *Landolt-Börnstein Tables* tries to be a comprehen-

sive publication of all the best values of data compiled from the world's literature in physics, chemistry, and technology. As an accommodation to its many English-speaking users, the *New Series of the Landolt-Börnstein Tables* is published bilingually (German and English).¹

The *Gmelin Handbook* published by the Gmelin Institute is probably the largest specialized compilation in West Germany. It also is probably the oldest work, having first been published in 1817 by Leopold Gmelin. The present edition, No. 8, was started in 1921 and is scheduled to be completed in about five years. Even after completion, however, it will continue to be supplemented.

The handbook is an exhaustive encyclopedic compilation, covering data on inorganic chemistry; physical chemistry; physics (including nuclear physics); analytical chemistry; colloidal chemistry; technology; crystallography; optical, electrical, and magnetic qualities of matter; mineralogy; geology; and metallurgy.

The *Gmelin Handbook* now comprises about 58 000 pages of text and figures. A classification scheme is used that facilitates the location of each compound or a combination of elements within the Gmelin series. This scheme is based on an arbitrary numerical sequence of elements—the so-called system numbers; it permits the systematic and comprehensive treatment of all major anionic groups for each cation-forming element in one place. Thus, all major compounds or properties of an element are classified in a volume pertaining to that element.

Like the *New Series of the Landolt-Börnstein Tables*, the *Gmelin Handbook* also accommodates its English-reading users by distributing a special brochure in English describing how its data are organized and classified. Further, since 1957, very detailed English headings and references are printed along the margins of the text. In addition to providing rapid and easy access to specific data, the bilingual headings and references serve as an excellent German-English glossary of terms.

The production of a work of this scope requires a large organization. The Institute's staff consists of about 80 scientists and an equal number of technical assistants

and auxiliary personnel. The staff has at its disposal all the major abstract journals, including those from Russia and China. In addition to these, more than 2 million archive cards are contained in its collection.

The Gmelin Institute maintains close ties with several American organizations, particularly the American Chemical Society; its U.S. office is located in Larchmont, N.Y.

The *Beilstein Handbook* deals solely with organic chemistry, and was first published in 1880. Within the next two decades and with the help of only one or two assistants, Beilstein prepared four volumes having a total of 6800 pages. Today, the *Beilstein Tables* comprise a Hauptwerk (main-work) of 28 volumes and three 28-volume supplements (all of which contain subvolumes). The main-work covers the literature to 1910 while the supplements cover the subsequent period to 1950. Altogether well over 100 000 pages have been published, and additional supplements will be published.

Ullmann's Technische Chemie, another of Germany's major technical handbooks, covers almost every aspect of modern chemical technology. The third and latest edition was initiated in 1951. To date, 17 volumes of this edition have been published—the latest in 1966. It will take several more years to complete the work; at present, this edition totals about 14 000 pages.

Besides these well known data compilation activities, Germany has a number of lesser known programs. One is the Documentation of Molecular Spectroscopy (DMS), which is based on the close cooperation of scientists in Great Britain and Germany. The DMS began publishing infrared spectral cards in 1956, and has since covered about 15 000 spectra.² The spectral cards are rim punched, slotted cards, which are coded according to various properties. To simplify sorting large numbers of spectral cards, a visual punched-card index was devised. Each index card has 5000 punchable positions. The serial number of each spectral card corresponds to one of the positions on the index card, while each index card corresponds to one of 211 possible properties encoded on the spectral cards. One issue of index cards covers a set of 5000 spectral cards. By combining the index cards of specific properties, the aligned holes in the cards indicate the serial numbers of those spectral cards that are coded for that particular combination of properties.

This same system is being used for two "current literature services" provided by DMS—one for infrared, Raman, and microwave literature; the other for nuclear magnetic resonance, electron paramagnetic resonance, and nuclear quadrupole resonance literature. Lists of about 600 pages are published every three months. Small-size visual punched-card indexes are included with the list, but will be replaced later by a large general index. In the future such literature services may be produced for mass spectroscopy and for emission spectroscopy, including atomic absorption and x-ray fluorescence.

A number of large German companies, particularly chemical and electrical companies, have developed their own systems of documenting critical data. One example is the Dornier Aeroplane factory which, with the help of IBM, has developed its own electronic "Dornier System" for storage and retrieval of important data. It uses a computer with a core memory of 16 000 words, and four long-time storage units, having 62 million words. The system was started with 45 chemical elements and their compounds, 25 physical properties and their combinations, and many other necessary data. It covers materials that can be bought commercially and includes the names of the suppliers throughout the world.

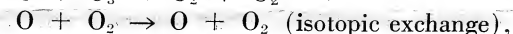
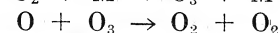
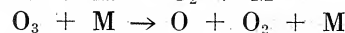
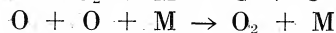
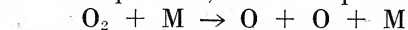
Unique to Germany are the DECHEMA material tables, which have the special purpose of compiling data on corrosion. Their 3200 pages provide data on the properties or reactions of 100 typical materials with more than 1000 different chemical substances.

A similar but smaller information system is edited by the Deutsche Kunststoff Institut of the Technical University of Darmstadt. It is managed by Professor Hellwege, editor of the *Landolt-Börnstein Tables*. This punched-card collection of data pertains to synthetic polymers.

Reaction Kinetics of Neutral Oxygen Species

NSRDS-NBS-20, *Gas Phase Reaction Kinetics of Neutral Oxygen Species*³ (49 pages; 45 cents), by Harold S. Johnston, is a review and re-analysis of the available chemical rate data for reactions among the neutral oxygen species O, O₂, and O₃. It is an up-to-date report on the status of the field.

Recommended expressions for rate coefficients (as a function of temperature) are developed for the reactions:



where M is an atom or molecule that serves as a "third body."

The analyses for each case are new. The available material for each reaction has been examined and that material considered still to be valid was used in developing the recommended values. In each case individual data points reported in journal articles are the basis for the analyses. All the data points used are tabulated in the monograph and are shown in figures, together with the recommended values.

Two of the results obtained deserve special mention. Mr. Johnston has shown that the many shock-wave studies of oxygen dissociation have produced data points that are consistent with each other; that is, they are samples of the same population but when they are viewed individually, the studies give widely different values. He has also made independent kinetic analyses for $\text{O}_3 + \text{M} \rightarrow \text{O}_2 + \text{O} + \text{M}$

NSRDS NEWS *continued*

and $O + O_2 + M \rightarrow O_3 + M$ and has shown that the ratio of these rates is in reasonable agreement with the thermodynamic data. The very slight discrepancy between the kinetic and thermodynamic analyses suggests a possible need for more calorimetric studies on ozone decomposition.

Reaction Rates for the H-O-N System

Another compilation of interest to chemical kineticists is *Reaction Rate Compilation for the H-O-N System*⁴ by Gilbert S. Bahn. This book is a reprinting of material that appeared in three parts in the periodical *Pyrodynamic*s, Vol. 5 (1967).

The work is a compilation of rate coefficients for reactions among atoms and simple molecules composed of only the atoms H, O, and N. Almost all of the reactions are elementary, one-step processes. The important species included are H, OH, H₂O, HO₂, H₂O₂, O, O₂, O₃, N, NH, NH₃, N₂H₄, and its fragments, HNO, HNO₂, HNO₃, and the nitrogen oxides.

The compilation is organized by reactions, with separate entries given for the forward and reverse reactions of a system. Under each reaction the material is organized by rate coefficient expression. For each of these values, the reference or references in which they are cited are given, together with remarks. These remarks cover the applicable temperature range, and the experimental method (where applicable); they often trace the values through the secondary references to their source.

Ample auxiliary material is provided to aid the user of the compilation. There is an index of reactions in which the order of reactants is permuted. An author index is provided. References are listed both in lists keyed to the compilation and to the *Pyrodynamic*s bibliography system. They are also listed by journal or by report issuer.

The coverage is extensive—it includes both published papers and reports. This compilation has as its goal a comprehensive listing of all available rate data for the reactions covered. Necessarily it includes many secondary references and statements of rates that are not based on experiment. The reader interested in experimental work will still have to sort through the material presented. The remarks indicate a careful examination of the source documents. The extensive mathematical, typographic, and bibliographic errors in the original papers should give casual users of rate data fair warning about the state of the literature. This is an exceptionally useful book for the student of reactions of atoms and light molecules.

Optical Atomic Spectra

The three volumes of NBS Circular 467, *Atomic Energy Levels*, by C. E. Moore, contain for each spectrum the bibliography that was used in compiling the data. A continuation of these bibliographies with the same format has been published in NBS Special Publication 306, *Bibli-*

ography on the Analyses of Optical Atomic Spectra, Section I, ¹H-²³V (80 pages; \$1), also by C. E. Moore.² It covers the literature published after NBS Circular 467 up to the present. The selection of references is restricted to those needed for the preparation of revised tables of atomic energy levels and multiplets.

CODEN Supplement

Supplement to CODEN for Periodical Titles, by J. G. Blumenthal, M. Karaman, and A. Peters, has been published in the ASTM Data Series DS 23A-SI.³ It is a supplement to the second edition of *CODEN for Periodical Titles*, ASTM DS 23A published in 1966. It adds 22 788 periodical titles and 2099 nonperiodicals to the 39 000 items presented in the second edition.

The CODEN system provides a form of abbreviation of serial titles that is suitable for both manual and machine use. A CODEN symbol⁶ consists of a five letter group identifying the series, the first four of which are often a mnemonic for the title. The fifth letter is a bookkeeping addendum. Example: NAFF-A, Natural Food and Farming (Atlanta, Tex.). The serials coded into the system are mainly in the science and technology area. At present, most of the periodicals in the physical sciences, medicine, and engineering are included; coverage in other areas is good.

The CODEN project is a continuing activity of ASTM and is carried out at the Franklin Institute in Philadelphia, Pa. At present the system includes some 75 000 titles and new material is being added at the rate of 2000 per month.

Neutron Cross Sections and Technology Proceedings

The Second Conference on Neutron Cross Sections and Technology was held in Washington, D.C., on March 4-7, 1968. Papers from this Conference have been published in two volumes as *Neutron Cross Sections and Technology, Proceedings of a Conference*, NBS Special Publication 299³ (1341 pp.; \$10.50 per set), edited by David T. Goldman. These volumes contain the texts of both the invited and contributed papers of the Conference. Topics include: The need for neutron data in science and technology; standard data and flux measurements; the determination of neutron cross sections by theoretical and experimental techniques; a presentation of recently measured data and their utilization in a variety of applications.

¹ See NSRDS News: Landolt-Bornstein Tables, NBS Tech. News Bull. 51, No. 6, 120-121 (June 1967).

² Information on DMS publications may be obtained from Butterworth & Co., 4/5 Bell Yard, Temple Bar, London, W.D.2, England.

³ Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, for the price indicated.

⁴ Published by Gordon and Breach, Science Publishers, New York, N.Y., 1968; price \$15.75.

⁵ Available from the American Society for Testing and Materials, Philadelphia, Pa., 1968, 469 pages; price \$45.

⁶ A full explanation of the CODEN System may be found in the article A Review of the ASTM CODEN for Periodical Titles, by Donald P. Hammer, Library Resources & Technical Services 12, No. 3, 359-365 (1968).